

```

1  #-*- coding: utf-8 -*-
2  """
3  Created on Tue Mar  5 10:48:44 2019
4
5  @author: Nate
6  """
7
8  import numpy as np
9  import matplotlib.pyplot as plt
10 import pdb
11
12 #fig2, axes2 = plt.subplots()
13
14
15 #####
16 #####
17 #defining constants
18
19 #number of trials
20 N = 100000
21
22
23 #α=0.2 to 2 in increments of 0.2
24
25 alpha = [i*.2 for i in range(1,11)]
26 rmax_list = [(3.2/alph) for alph in alpha]
27 r0 = np.array([0.01,0,0])
28 energy = []
29 std_dev = []
30
31
32
33 #sigma = [4*i for i in alpha]
34 #rmax = 1/(2*alpha)
35
36
37
38
39 #####
40 #####
41 #defining functions
42
43
44 def get_delta_r(rmax):
45     delta_r =
46         np.array([rmax*(np.random.uniform()-.5),rmax*(np.random.uniform()-.5),rmax*(np.random
47             .uniform()-.5)])
48     return(delta_r)
49
50 #evaluate ratio
51 def evaluate_ratio(r, delta_r):
52     global count
53     A = np.exp(-2*alpha[i]*np.linalg.norm(r))
54     B = np.exp(-2*alpha[i]*np.linalg.norm(r+delta_r))
55     ratio = B/A
56
57     if ratio > np.random.uniform():
58         count+=1
59         return(True)
60     else:
61         return(False)
62
63 def generate_point(r, delta_r):
64     if evaluate_ratio(r, delta_r) == True:
65         return(r+delta_r)
66     else:

```

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66         return(r)
67
68
69 #####
70 #####
71
72
73
74 for i in range(len(alpha)):
75
76     #generating points
77     r = np.array([r0])
78     count = 0
79     en = 0
80
81     for j in range(N):
82         #r2=np.random.exponential(.5/alpha[i])
83         #en += -alpha[i]**2 + alpha[i]/np.linalg.norm(r2) - 1/np.linalg.norm(r2)
84
85         #pdb.set_trace()
86         r = np.append(r, [generate_point(r[len(r)-1], get_delta_r(rmax_list[i]))], axis
87                         = 0)
88         en += -(alpha[i]**2)/2 + alpha[i]/np.linalg.norm(r[j]) - 1/np.linalg.norm(r[j])
89
90     print(rmax_list[i], 'accepted: ', count, 'rejected: ', N-count)
91     print('Acceptance Ratio: ', count/N)
92     energy.append(en/N)
93
94
95     to_sum = 0
96     for j in range(N):
97         to_sum += (- (alpha[i]**2)/2 + alpha[i]/np.linalg.norm(r[j]) -
98                    1/np.linalg.norm(r[j]) - energy[i])**2
99
100
101     std_dev.append(np.sqrt(to_sum)/np.sqrt(N))
102
103     '''
104     if i == 1:
105         axes2.hist([np.linalg.norm(i) for i in r], bins = 100, normed = True)
106         axes2.plot([n*.1 for n in range(0,3000)], [2*alpha[i]*np.e**(-2*alpha[i]*n*.1) for n in range(0,3000)])
107     '''
108
109 print(energy)
110
111 #####
112 #####
113 #Plotting
114
115 fig1, axes1 = plt.subplots()
116
117 #axes1.scatter(alpha, [3/2*num-2**(3/2)/(np.pi**.5)*num**.5 for num in alpha])
118 #axes1.scatter(8/(9*np.pi), [3/2*(8/(9*np.pi))-2**(3/2)/(np.pi**.5)*(8/(9*np.pi))**.5])
119 #axes1.plot(alpha, energy)
120 axes1.errorbar(alpha, energy, yerr=std_dev, fmt='o', linestyle = '-')
121 axes1.plot(alpha, [(num**2)/2-num for num in alpha])
122
123 axes1.set_ylabel('Energy')
124 axes1.set_xlabel('alpha')
125 axes1.set_title("Energy vs alpha", va='bottom')
126
127
128 plt.show()

```